Special Session 64: Analysis of PDEs and Particle Systems: From Life Sciences, Economics and Materials Science

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The focus of this special session is on the modeling and analysis of continuous and discrete scenarios relevant to selected real-world applications.

Besides well-posendess studies of nonlinear PDEs and particle systems arising from materials and life science, the session also includes presentations on averaging processes in porous media, mathematical homogenization, statistical mechanics of particle systems, large-time behavior of solutions, multiscale dynamics of pedestrian flows.

Particularly, mathematical modeling for macro-economics exposed to extreme conditions (e.g. natural disasters like tsunamis, earthquakes etc.) will be open for discussions.

One-dimensional concrete carbonation problem with nonlinear Henry's law

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In this talk we consider a free boundary problem as a mathematical model for concrete carbonation on a one-dimensional domain $(0, \infty)$. The problem is to find a carbonation front $x = s(t) > 0$ and concentrations u and v of carbon dioxide in water and air regions, respectively. In our previous works we consider the linear function $f(u, v) = a(bv - u)$ as a mathematical description for contribution of Henry's law, where a and b are positive constants. Now, we suppose that $f(u, v) = \phi(bv - u)$, where ϕ is a continuous and increasing function on R. The aim of this talk is to show a large time behavior of the carbonation front.

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Stochastic nucleation and growth of particle clusters

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The binding of individual components to form composite structures is a ubiquitous phenomenon within the sciences. Within heterogeneous nucleation, particles may be attracted to an initial exogenous site: the formation of droplets, aerosols and crystals usually begins around impurities or boundaries. Homogeneous nucleation on the other hand describes identical particles spontaneously clustering upon contact. Given their ubiquity in physics, chemistry and material sciences, nucleation and growth have been extensively studied in the past decades, often assuming infinitely large numbers of building blocks and unbounded cluster sizes. These assumptions also led to the use of mass-action, mean field descriptions such as the well known Becker Doering equations. In cellular biology, however, nucleation events often take place in confined spaces, with a finite number of components, so that discrete and stochastic effects must be taken into account. In this talk we examine finite sized homogeneous nucleation by considering a fully stochastic master equation, solved via Monte-Carlo simulations and via analytical insight. We find striking differences between the mean cluster sizes obtained from our discrete, stochastic treatment and those predicted by mean field treatments. We also consider heterogeneous nucleation stochastic treatments, first passage time results and possible applications to prion unfolding and clustering dynamics.

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Global effect of local anisotropic interactions in crowd dynamics

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Many models for describing the behaviour of people in a crowd start from a microscopic point of view, i.e. at the individual's level. These models are mainly inspired by those used in physics, statistical mechanics etc. for studying particles systems (grains, colloids, molecules, etc.). In contrast to particles, people have well-defined front and back sides. Consequently, mutual interactions are highly influenced by the angle under which individuals perceive each other. Up to now, this kind of anisotropy was explored in simulations, but analytic understanding is lacking.

We use a model formulated at the macroscopic level (i.e. the crowd is considered to be a continuum), in which we prescribe the structure of the velocity field. It basically consists of a "desired velocity" which is perturbed by a "social velocity" term, due to the presence of other people. In this talk, I explain our model and the way in which we include anisotropy due to visual perception. Furthermore, I give a flavour of the large-scale effects that inherently arise.

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Swarm dynamics and equilibria for a nonlocal aggregation model

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We consider the aggregation equation $\rho_t - \nabla \cdot (\rho \nabla K * \rho) = 0$ in $\mathbb{R}^n$, where the interaction potential K models short-range repulsion and long-range attraction. We study a family of interaction potentials with repulsion given by a Newtonian potential and attraction in the form of a power law. We show global well-posedness of solutions and investigate analytically and numerically the equilibria and their global stability. The equilibria have biologically relevant features, such as finite densities and compact support with sharp boundaries.

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Abstract theory of the variational inequality and the Lagrange multiplier

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In this talk, we discuss the well-posedness of the variational inequality of the heat equation with the time-dependent constraint. This kind of problem was treated by E. Ginder (2010) as the heat equation with the time-dependent volume constraint, and the references therein. Using the Lagrange multiplier, the initial and Dirichlet boundary value problem was formulated. The objective is to obtain the abstract theory of the variational inequality and the Lagrange multiplier. Moreover under the assumption weaker than Ginder's one the well-posedness is obtained. Finally, using the relationship between our variational inequality and its Lagrange multiplier, we also discuss the regularity of the solutions.

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Solvability of the tumor invasion model

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In this talk, we discuss for solvability of the tumor invasion models which is Chaplain-Anderson type having some diffusion. Similar to the results so far, This result has been used by Quasi-Variational inequalities. Quasi-variational inequalities can be an abstract representation of the system with a strong dependency. Also I talk about the abstract formulations.

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Revival full model of human and economic activities in disaster regions

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After disasters such as earthquake, tsunami, typhoon etc., we have to face a lot of serious problems, for instance, environment destroy for life and economic collapse and dispersion of habitants. It is quite important to recover human and economic activities in the disaster regions as soon as possible, by providing suitable supports for them. In general it takes a long time (10 or 20 years more) to recover the complete environment which is the basis of our life. In any case, we have to restart our life in incomplete circumstances. Moreover, at the same time one has to start adequate reorganization of production systems in order to renew the economical situation in disaster regions. We know many mathematical models dealing with the evolution of human activity and the economic growth, independently each other. However, in disaster regions the both aspects should be treated simultaneously on a correlative connection, although the corresponding model is much more complicated than the usual ones. In this talk we propose a simplified system of ordinary differential equations, which we call the revival full model of human and economic activities in disaster regions.

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On a mathematical model of moisture transport with a time-dependent porosity in concrete carbonation process

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In this talk we consider a mathematical model of moisture transport in concrete carbonation process in three dimensional case. This model is a diffusion equation with a hysteresis operator indicating the relationship between the relative humidity and the degree of saturation. Also, this equation has a porosity which contains a non-local term in a coefficient of the time derivative of the unknown function and a perturbation. In this talk we prove the existence of a solution of a initial boundary value problem of this model.

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Solutions to the Kohn-Sham model for heavy atoms

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The Density Functional Theory (DFT) of Kohn and Sham has emerged as the most widely-used method of electronic structure calculation in both quantum chemistry, condensed matter physics and materials science.

We study the standard and extended Kohn-Sham models for quasi-relativistic N-electron Coulomb systems describing heavy atoms; that is, systems where the kinetic energy of the electrons is given by the quasi-relativistic operator

$$\sqrt{-\alpha^{-2}\Delta_{x_n}+\alpha^{-4}}-\alpha^{-2}.$$

For spin-unpolarized systems in the local density approximation, we prove existence of a ground state (or minimizer) provided that the total charge Z_{tot} of K nuclei is greater than $N-1$ and that Z_{tot} is smaller than a critical charge $Z_{\text{c}} = 2\alpha^{-1}\pi^{-1}$. The proof is based on the concentration-compactness approach to locally compact variational problems involving non-local operators.

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Mathematical modeling for brewing process of Sake and its analysis

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"Sake" is brewing liquor with using fermenting technique so-called "Multiple parallel fermentation". "Multiple parallel fermentation" is one of the most difficult way of fermentation. We have a few data about brewing process of Sake because "Multiple parallel fermentation" is too complicated. We propose a mathematical modeling for brewing process of Sake to analyze the phenomena, and to construct brewing, forecast, and control techniques from mathematical and engineering point of view. We'll introduce this modeling and discuss existence some solutions for our modeling.

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Qualitative analysis of homogenization.

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In this talk we will discuss two research avenues for the qualitative analysis of homogenization results: 1. The role of boundary layer correctors in the study of error estimates 2. The use of novel spectral decomposition results for the local representation of multi-scale problems solutions leading to global macro-scale approximation algorithms for the initial micro-scale phenomena. In this talk we will mainly present our ideas in the context of the elliptic homogenization for general problems with non-smooth coefficients and discuss the possible extensions of our results to the time-dependent case and to the case of variable geometries.

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Elastic properties of a exoskeleton and homogenization of plywood structures

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Many biological or industrial composite materials comprise non-periodic microscopic structures, for example fibrous microstructure with varied orientation of fibers in exoskeletons, in polymer membranes and in industrial filters, or space-dependent perforations in concrete. An interesting and important for applications special case of non-periodic microstructures is so called locally-periodic microstructure, where spacial changes of the microstructure are observed on the scale smaller than the size of the considered domain but larger than the characteristic size of the microstructure. The notion of locally-periodic two-scale convergence is introduced. As admissible test functions we consider the functions of two variables such that they periodicity with respect to the second (microscopic) variable may depend on the fist (macroscopic) variable. The developed theory is applied to derive effective macroscopic equations for a linear elasticity problem defined in a domain with a plywood structure, a prototypical pattern found in the exoskeleton. The plywood structure is characterised by the superposition of gradually rotated planes of parallel aligned fibres.

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Continuous dependence of entropy solutions to strongly degenerate parabolic equations with discontinuous coefficients

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Strongly degenerate parabolic equations are regarded as a linear combination of the time-dependent conservation laws (quasilinear hyperbolic equations) and the porous medium type equations (nonlinear degenerate parabolic equations). Thus, these equations have both properties of hyperbolic equations and those of parabolic equations and describe various nonlinear convective diffusion phenomena such as filtration problems, Stefan problems and so on. In this talk we consider the strongly degenerate parabolic equations with discontinuous coefficients. In particular, we focus our attention on the continuous dependence of entropy solution to such equations.

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Optimal control problem of positive solutions to second order impulsive differential equations

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In this talk, we focus on optimal control problem of the positive solution to second order impulsive differential equations. We show the existence and uniqueness of positive solutions to our problem for each given control functions. Also, we consider the control problem of positive solutions to our equations. Then, we prove the existence of an optimal control that minimizes the nonlinear cost functional. Moreover we consider the special case of our problem, and then, we given the necessary condition of optimal control.

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